Adaptive Finite Elements with Local ALE for Modeling Turbulent Reactive Flow in Engines with Injection

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LANL and collaborators are facilitating the effort for predictive internal combustion engine modeling. We are developing an *hp*-adaptive finite element methods (FEM) software that provides a high degree of accuracy and solution robustness. This FEM projection method, using a predictor-corrector scheme (PCS), has excellent capability over all flow regimes. The system is applicable to Newtonian and non-Newtonian fluids, turbulent reactive flows with sprays, and using a new local Arbitrary Lagrange-Eulerian (ALE) method for immersed moving parts.

These algorithms are capable of representing the physics within an engine. Theoretical Division resources and its collaborators provide software that many designers and researchers can use directly for engine simulation or may alter using their own models. KIVA software is in use worldwide by hundreds of universities and dozens of corporations involved in research, engine design, and manufacturing. We are working to deliver a more predictive capability to help in the understanding of combustion engines, thereby providing for greater efficiency and lower unwanted emissions.

LANL is continuing to develop advanced numerical methods that can be used in combustion and propulsion. We provide software that others may use directly or that they may alter with various models such as sophisticated chemical kinetics, different turbulent closure methods, or different fuel injection systems.

Current users are worldwide, from individuals and small research institutions to large corporations. We expect to deliver a more predictive and robust modeling capability. When put to use by researchers and corporations, we hope to better understand the complicated chemistry and physics associated with internal combustion engines. Greater efficiency is expected to result, helping to meet the newest US efficiency and pollution requirements for 2015, the aggressive requirements for 2020, and those in the future.

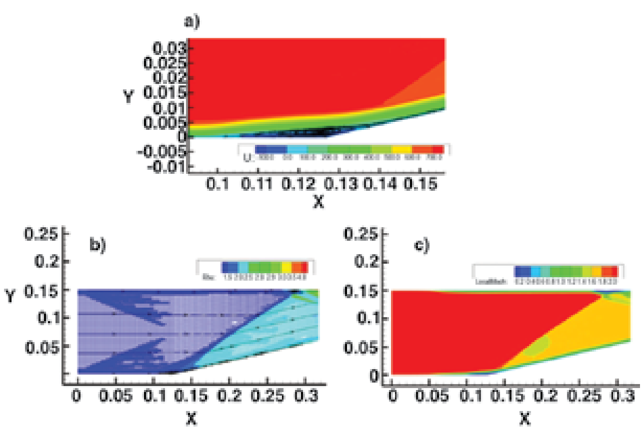

Fig. 1. Mach 2.25 steady-state flow properties for 2D supersonic viscous flow through a 18° compression ramp. (a) Recirculation, shock separation (distance in meters), (b) Density, (c) Local mach number.

When considering the development of algorithms and the significant effort involved to produce reliable software, it is often best to create algorithms that are more accurate at a given resolution only where and when it is required. We began developing a new KIVA engine/combustion code with this idea in mind [1]. This new construction is a Galerkin FEM approach that utilizes conservative momentum, species, and energy transport. Our system uses a Petrov-Galerkin (P-G) and coupled-pressure stabilization [2].

A projection method is combined with higher-order polynomial approximation for model-dependent physical variables (*p*-adaptive) along with grid enrichment (locally higher grid resolution—*h*-adaptive). Overset grids are used for actuated and immersed moving parts to provide more accurate and robust solutions in the next generation of KIVA. The scheme is particularly effective for complex domains such as engines.

The *hp*-adaptive FEM is, at a minimum, second-order accurate in space and third-order for advection terms, but becomes higher order where required as prescribed by the adaptive procedures [2]. The *hp*-adaptive method employs hierarchical basis functions, constructed on the fly as determined by a stress-error measure [3].

The *h*-adaptive method, along with a conservative P-G upwinding technique, accurately captures shocks. Figure 1 shows viscous supersonic Mach 2.25 occurring over an 18° compression ramp with the shock captured using adaptation. The velocity compares to experimental data as shown in Fig. 2 [4]. Differences are related to the k-ω turbulence closure model–other models can capture the boundary layer more precisely but are more costly and can be less generic. The recirculation zone shown in Fig. 1(a) is an affect of the adverse pressure gradient developing in the boundary layer at the incline and is in agreement with the experimental data. The data only shows absolute speed, not direction. Taking this into account, the velocity for the k-ω model is

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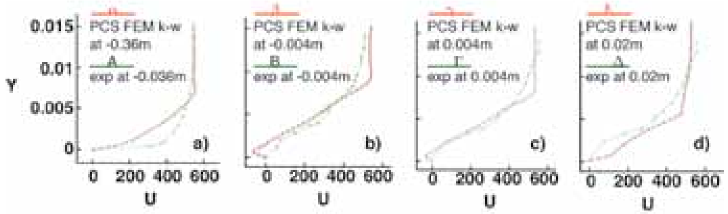

Fig. 2. U (mean velocity) in bottom boundary layer using k-ω model. Comparison to data at two locations: Upstream(-) and downstream(+) of the ramp (a) -0.004m, (b) +0.004m, (c) +0.004m, and (d) +0.036m.

closer to the actual data than indicated in the Fig. 2(a) and (b).

Figure 3 shows both 2D and 3D subsonic/transonic flow over a NACA 0012 airfoil that also agrees with known solutions and data. This system incorporates a method for the measurement of the error in the discretization, and adjusts the spatial accuracy to minimize the error or bring it under some specified amount while minimizing the total number of nodes or elements in the domain.

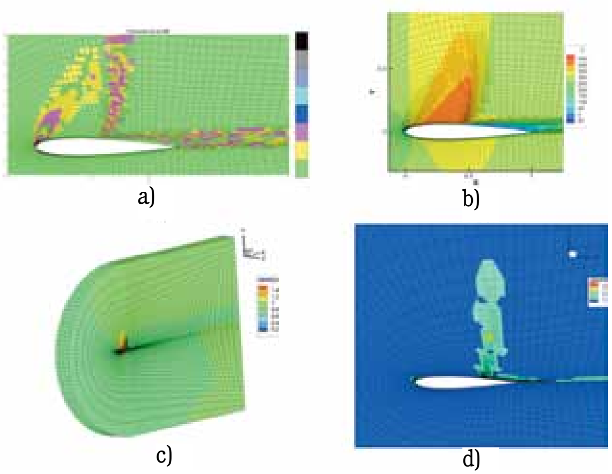

Fig. 3. Transonic flow over an NACA 0012 airfoil at 4° AOA, using hp-adaptive PCS FEM: (a) 2D hp grid with colors showing order of approximation. (b) 2D U component of velocity. (c) 3D Mach numbers. (d) 3D hp grid with colors showing order of approximation.

The FEM method, when coupled with the spray models, provides a more accurate representation of droplet interaction with the conveying fluid and walls compared with the finite volume method used in the original version of KIVA. Because the FEM method allows for a continuous representation of phase-space, grid-scale accuracy can be applied everywhere. Problems with coarse grids influencing the spray are related only to the solution accuracy–the spatial representation of the spray model is therefore convergent. The KIVA multi-component spray model, a method based on the algorithm developed by Dukowicz [5] and expanded by Torres et al. [6] for break-up, agglomeration, and surface films, is being installed in the *hp*-FEM PCS solver. In Fig. 4, diesel fuel is shown injected into a duct having developed flow and an inlet speed of 25 m/s (Mach 0.061) with an inlet Reynolds number of

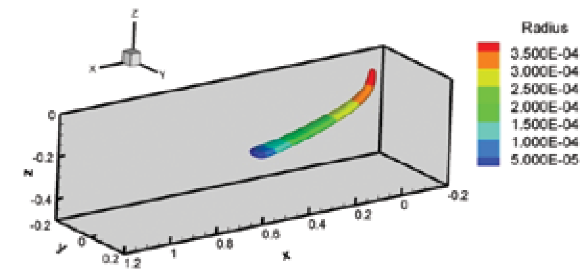

Fig. 4. Injection and spray modeling test case for PCS FEM. Diesel spray modeling: droplet breakup, agglomeration, and complete evaporation.

~1,204,000. The droplet radius is changing as a function of convective and diffusive heat and mass transfer, evaporating the droplets. Heat conduction within the droplet, collisions, and agglomeration occurs as the droplets are transported. Each parcel can have around 500 droplets (for 3D). The number of parcels/droplets is determined by the flow rate and injector size and is often in the neighborhood of 4000 parcels for about 200,000 droplets being represented.

Development of an *hp*-adaptive PCS FEM for all four regimes has been achieved. Compressible flow validation continues along with the implementation of the chemistry and spray models and new turbulence models, including large eddy simulation (LES) in wall-bounded domains. This projection method is a new solution algorithm for advancing the accuracy, robustness, and range of applicability of the KIVA combustion software suite. The system is higher-order both spatially and temporally yet provides a minimal amount of computational effort.

We have completed a local ALE technique for 2D that has second-order spatial convergence of error and will never tangle the grid [7]. The local ALE scheme uses overset grids for immersed parts described by their boundaries, which overlay the fluid grid. The moving parts within the fluid are not taken into account during the grid generation process. Hence, ports and cylinder portions of the grid are continuously represented. Because of this feature, the system allows CAD-to-grid in nearly a single step, providing nearly automatic grid generation.

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